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S8 – S24: Spectra of Synthetic Compounds

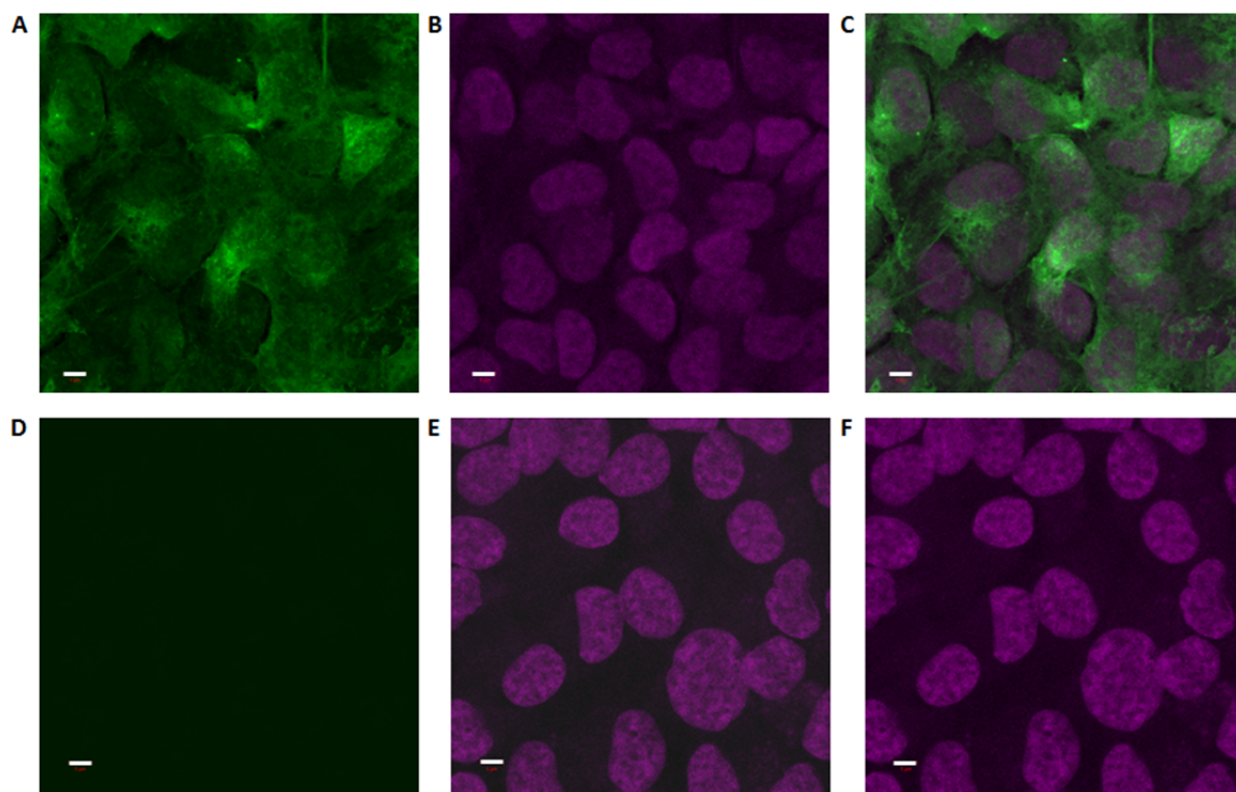


Figure S1. Enlarged version of fluorescence images of cell labeling by probe **1a**. Human T-24 cancer cells were treated with clickable Cy3 fluorophore **8** in the presence (**A-C**) or absence (**D-F**) of probe **1a**. **A&D**: Cy3 channel (green), **B&E**: DAPI channel (magenta), **C&F**: Merged images. Scale bars (white) indicate 5 μm .

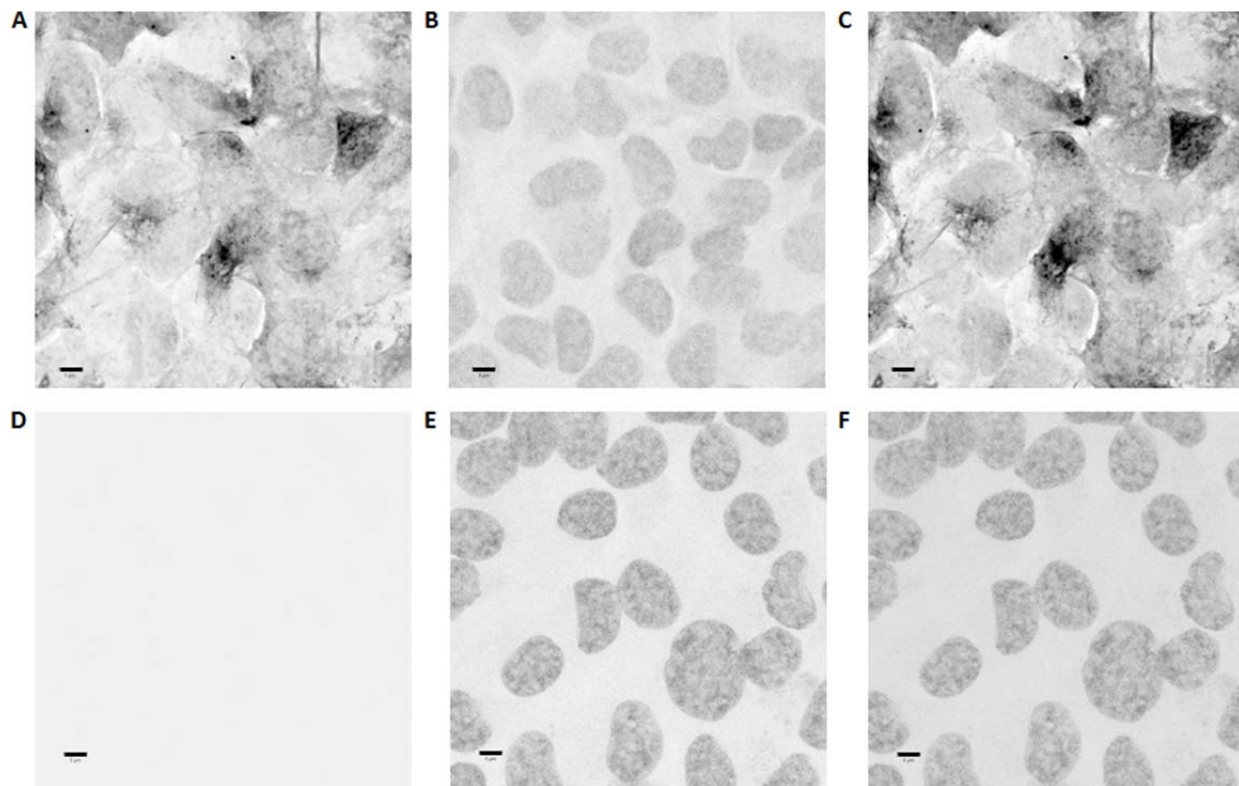


Figure S2. Enlarged and greyscaled version of fluorescence images of cell labeling by probe **1a**. Human T-24 cancer cells were treated with clickable Cy3 fluorophore **8** in the presence (**A-C**) or absence (**D-F**) of probe **1a**. **A&D**: Cy3 channel, **B&E**: DAPI channel, **C&F**: Merged images. Scale bars (black) indicate 5 μm .

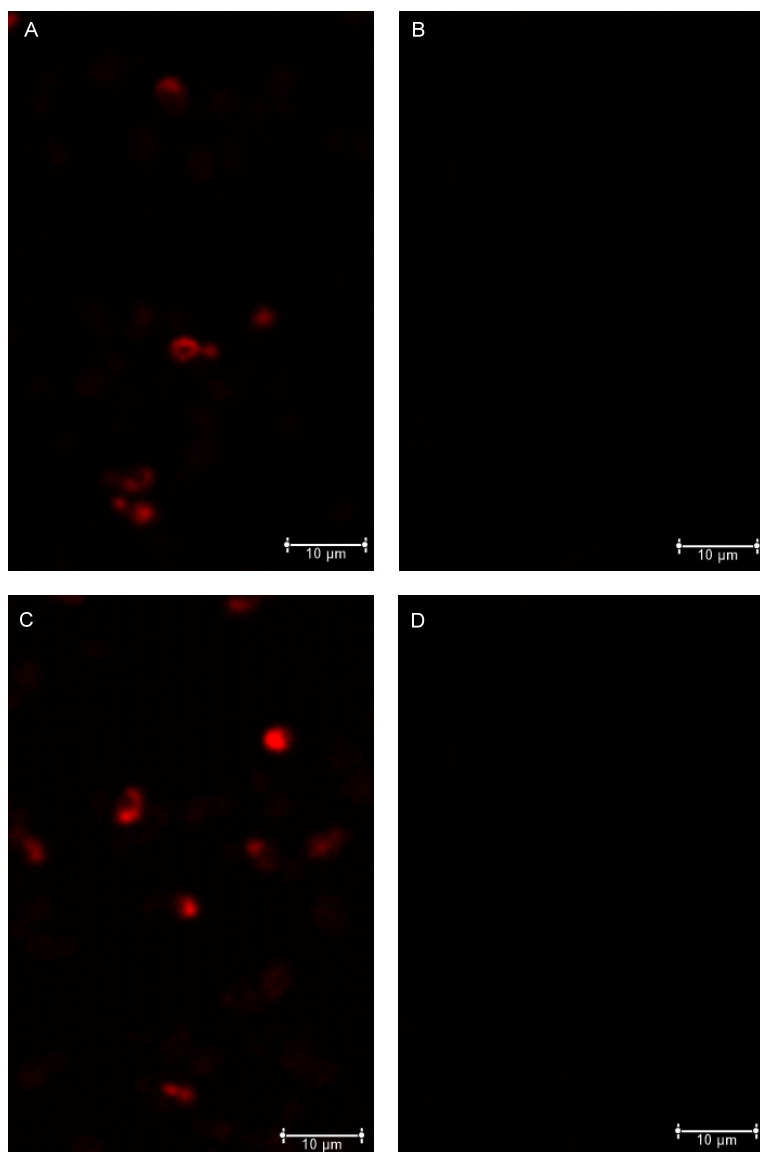


Figure S3. Enlarged version of fluorescence imaging results using *C. albicans* cells. Treatment with **8** in the presence or absence of **1a** was performed with WT cells (A and B, respectively, Cy3 channel (red)) and *itr1ΔΔ* cells (C and D, respectively). Scale bars indicate 10 μm.

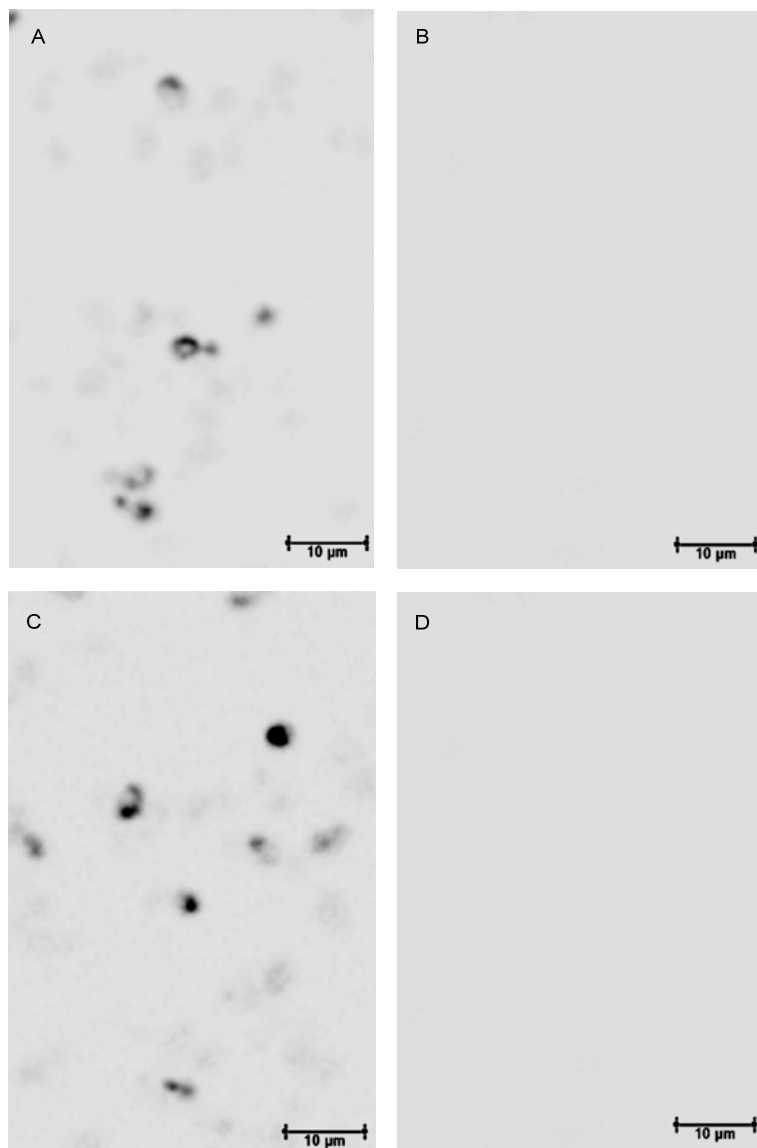
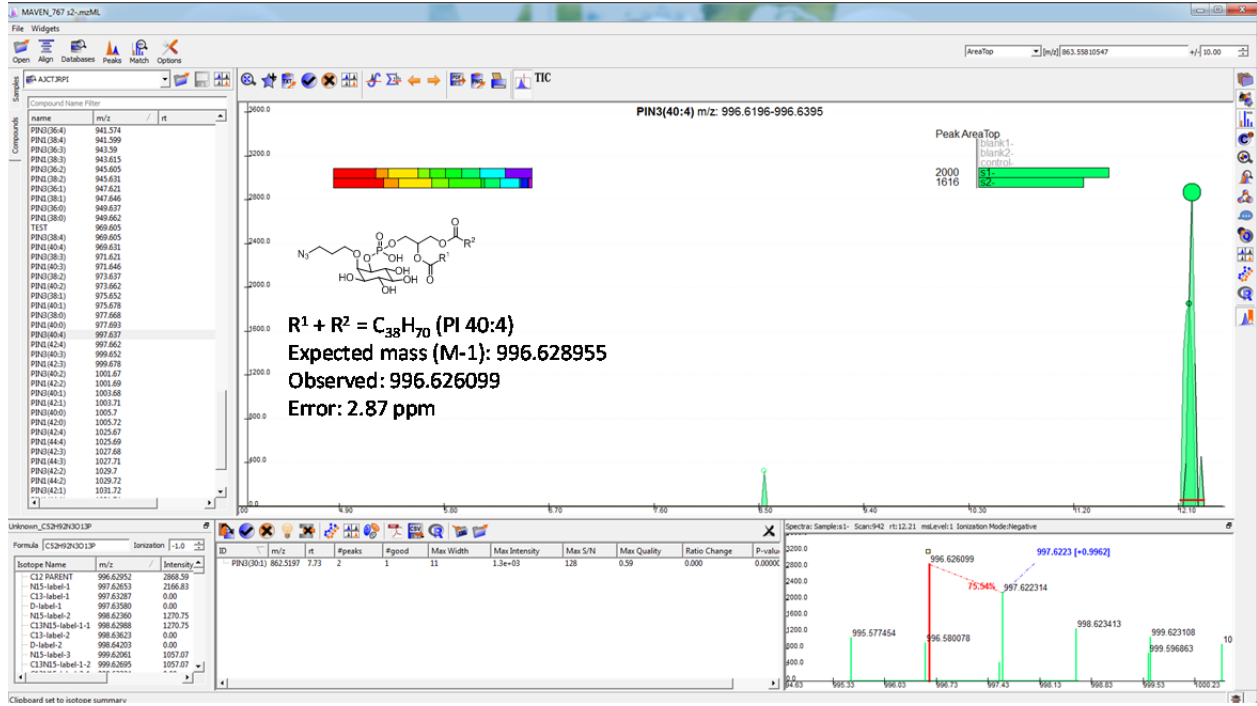
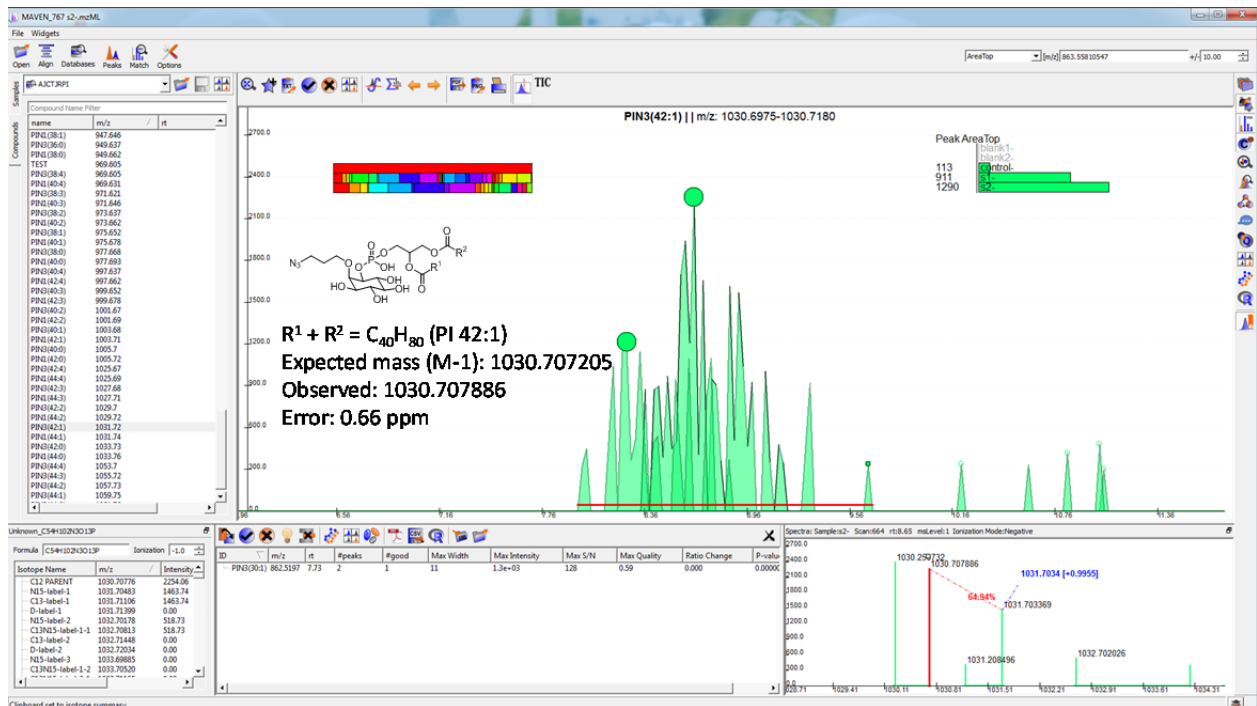


Figure S4. Enlarged and greyscaled version of fluorescence imaging results using *C. albicans* cells. Treatment with **8** in the presence or absence of **1a** was performed with WT cells (A and B, respectively) and *itr1*ΔΔ cells (C and D, respectively). Scale bars indicate 10 μm.

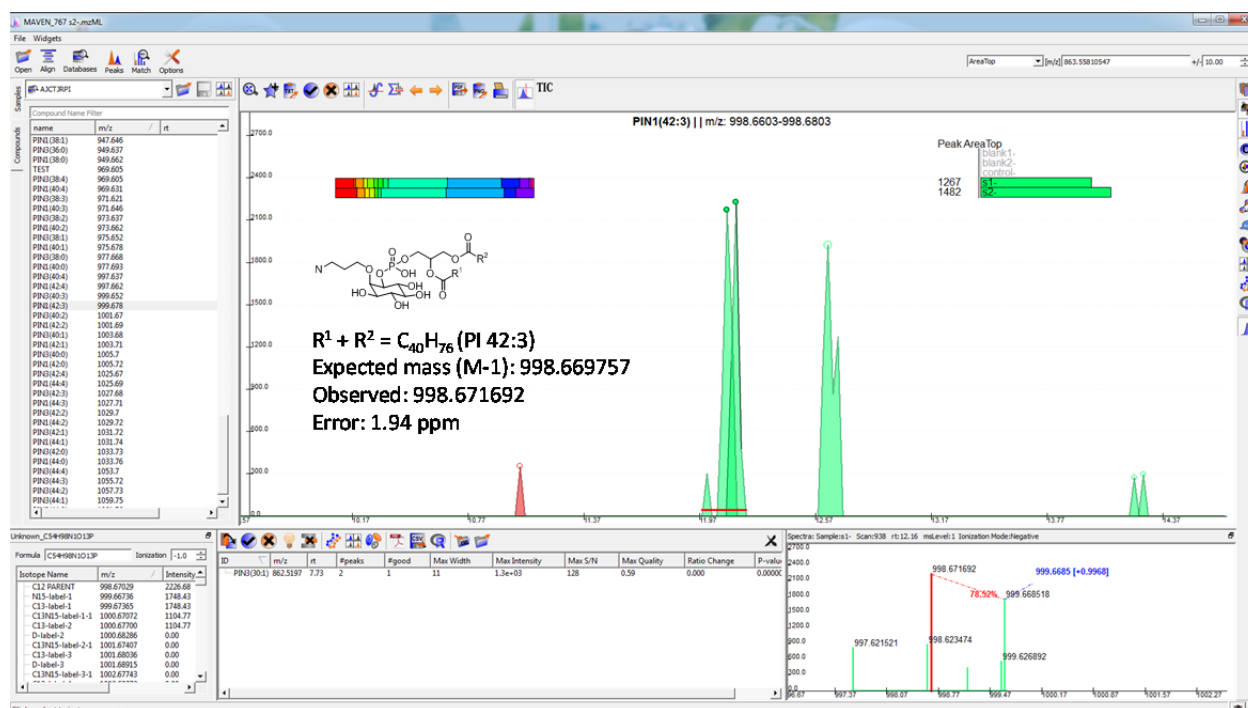
A



B



E



F

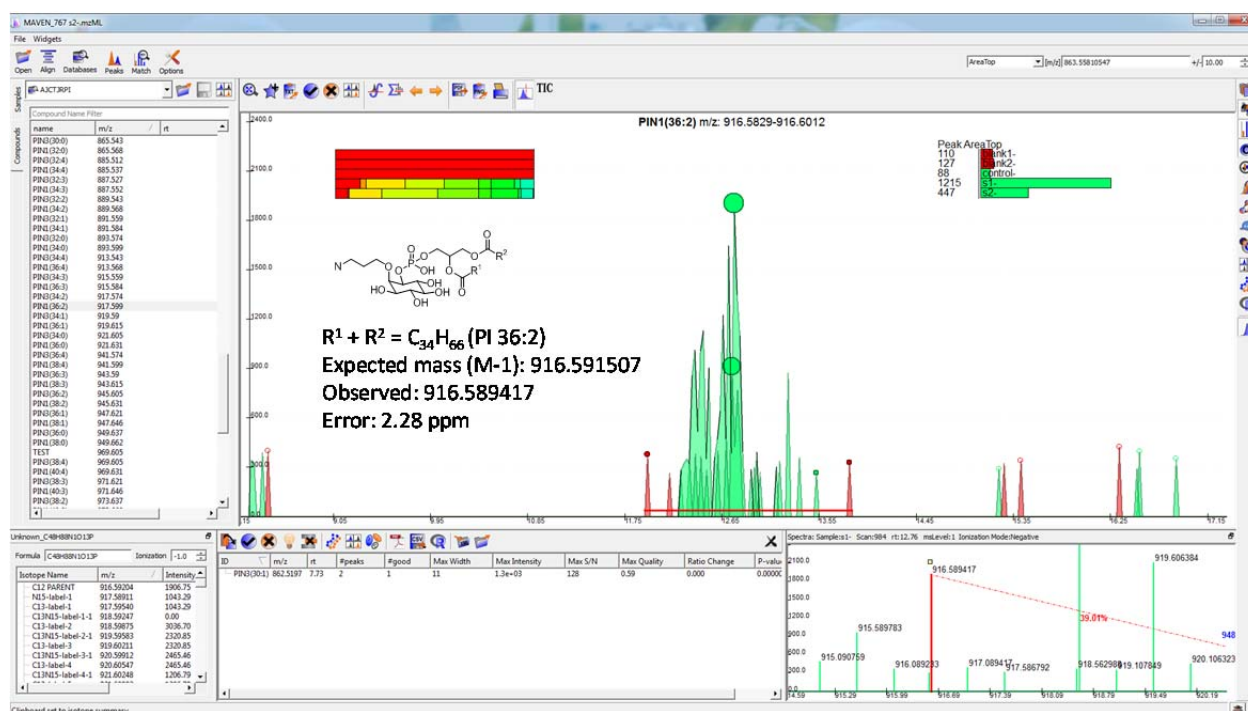
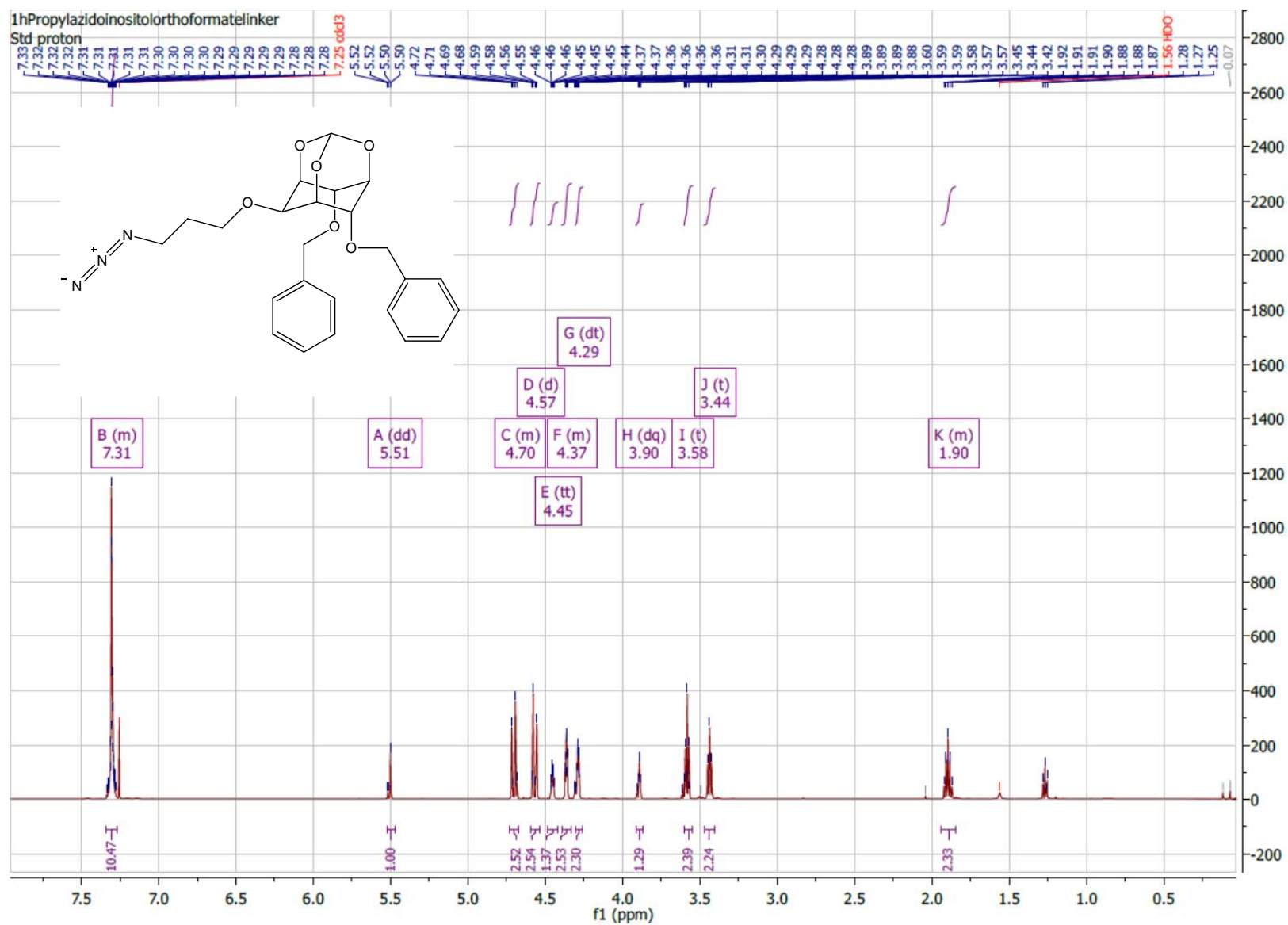
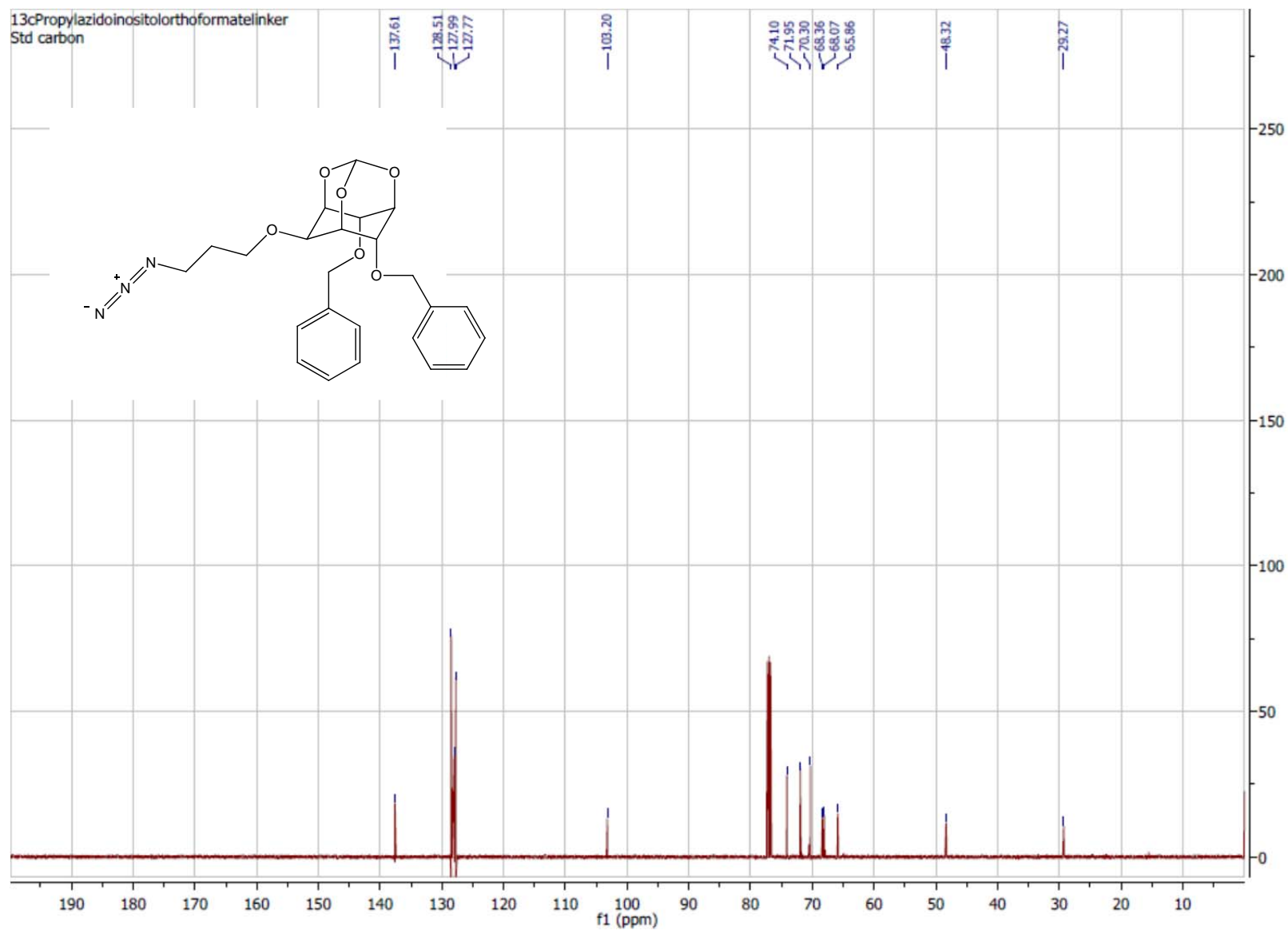


Figure S5. Representative mass spectra detected by liquid chromatography mass spectrometry (LCMS) for click-tagged products of *myo*-inositol probe **1a**. Structures are shown that match detected mass peaks. The x-axis shows the retention time from LC separation while the y-axis indicates the areas of peaks containing the relevant mass ion based on ion counts. The colored inset plots these peak areas and depicts two replicate samples (s1 and s2), a control sample of cells lacking probe **1a**, and blank samples. These spectra resulted from LCMS runs in negative mode on a Thermo Scientific Q Exactive Hybrid Quadrupole-Orbitrap Mass Spectrometer.

¹H NMR of compound 4



¹³C NMR of compound 4

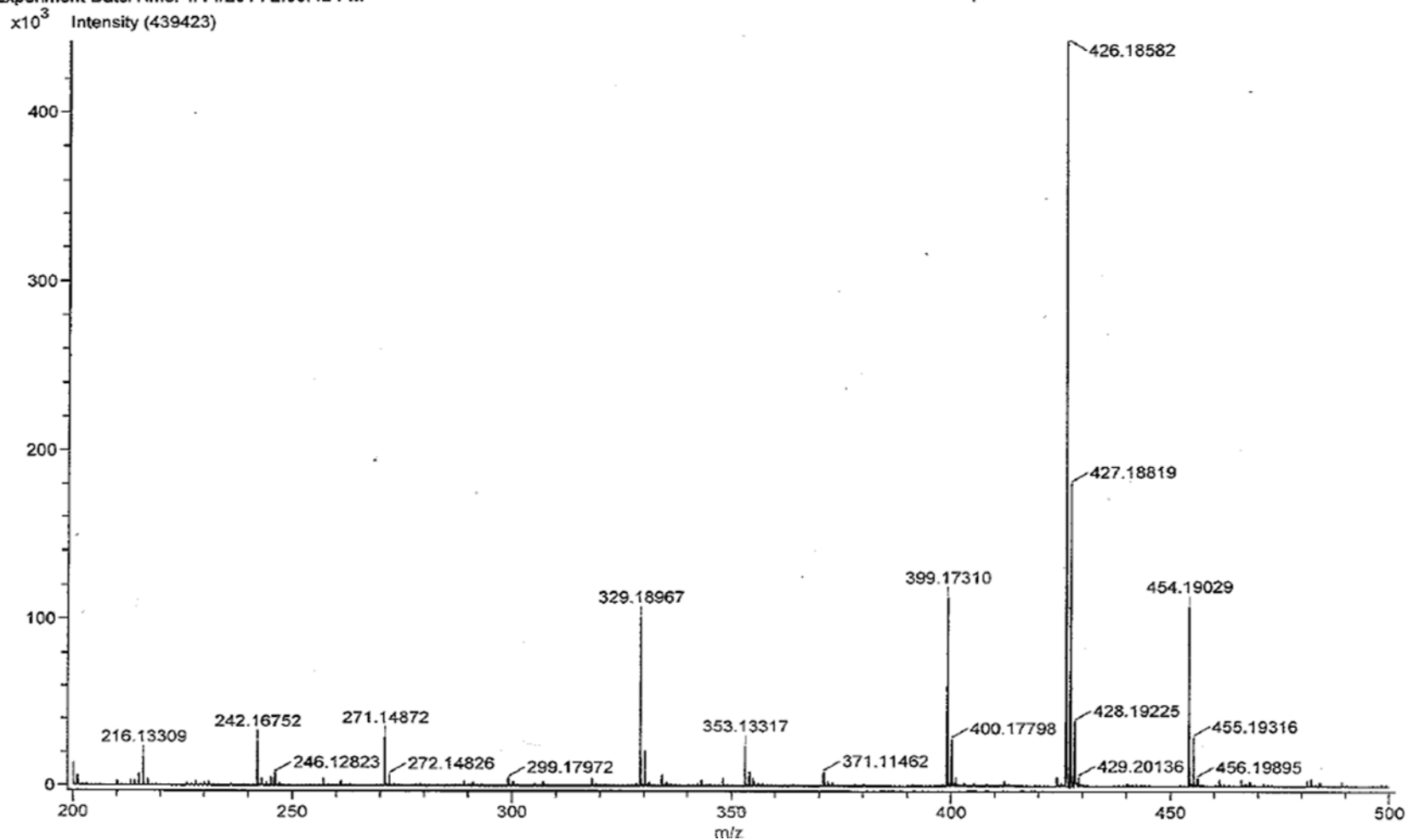


ESI-MS of compound 4

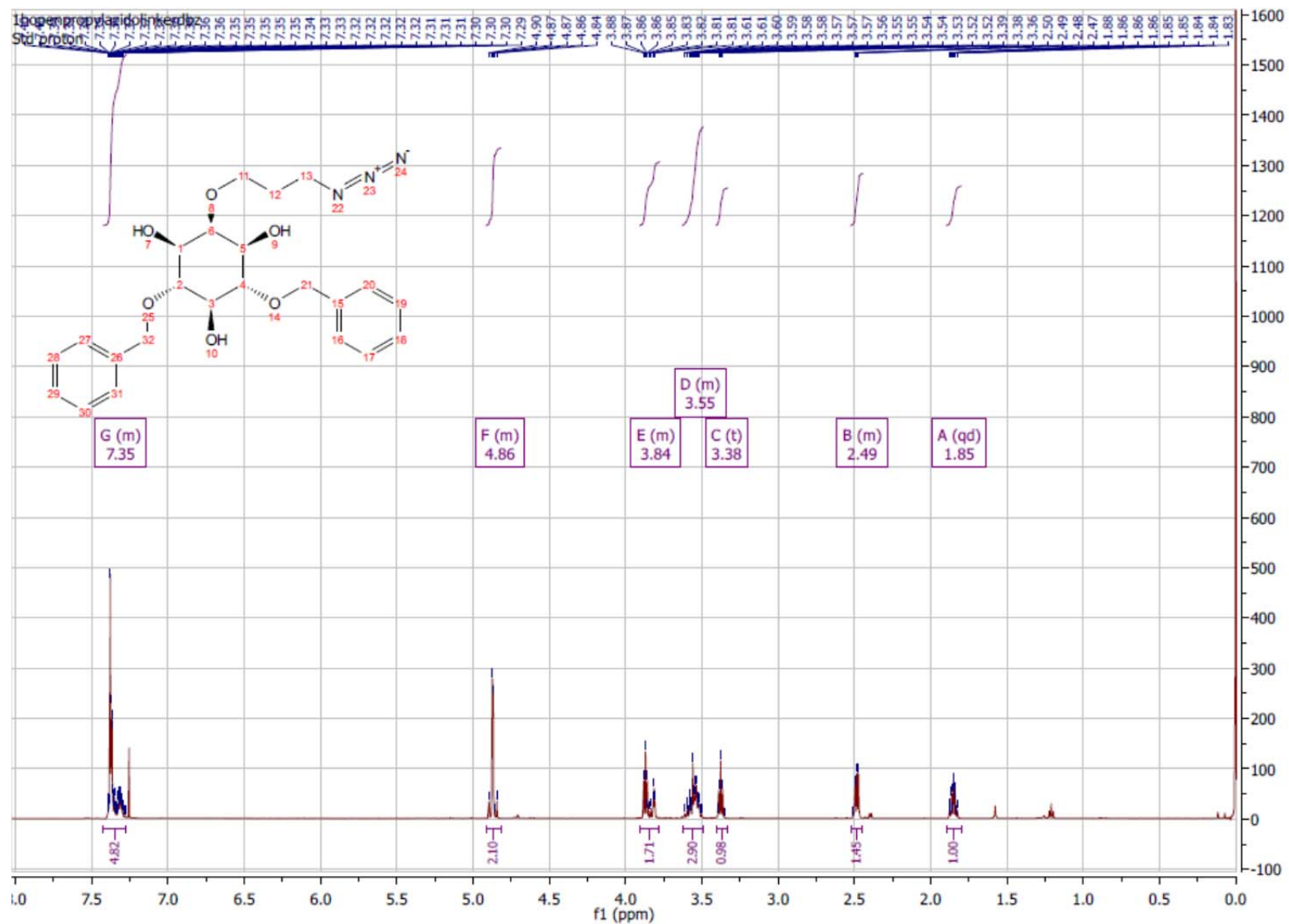
Acq. Data Name: 140114_Best_tricks_propylazidoinsorthoformdbz
Internal Sample Id:
Ionization Mode: ESI+ Orifice1 Volt Sweep: 30V
MS Calibration Name: PEG_DART_1000 Acquired m/z Range: 200.0..500.0
Reduction History: Correct Base[5.0%];Average(MS[1] 0.902..0.962)
Experiment Date/Time: 1/14/2014 2:00:42 PM

Spec. Record Interval: 1.0[s]
Ring Lens Volt: 10[V]
Time of Maximum: 0.926[min]

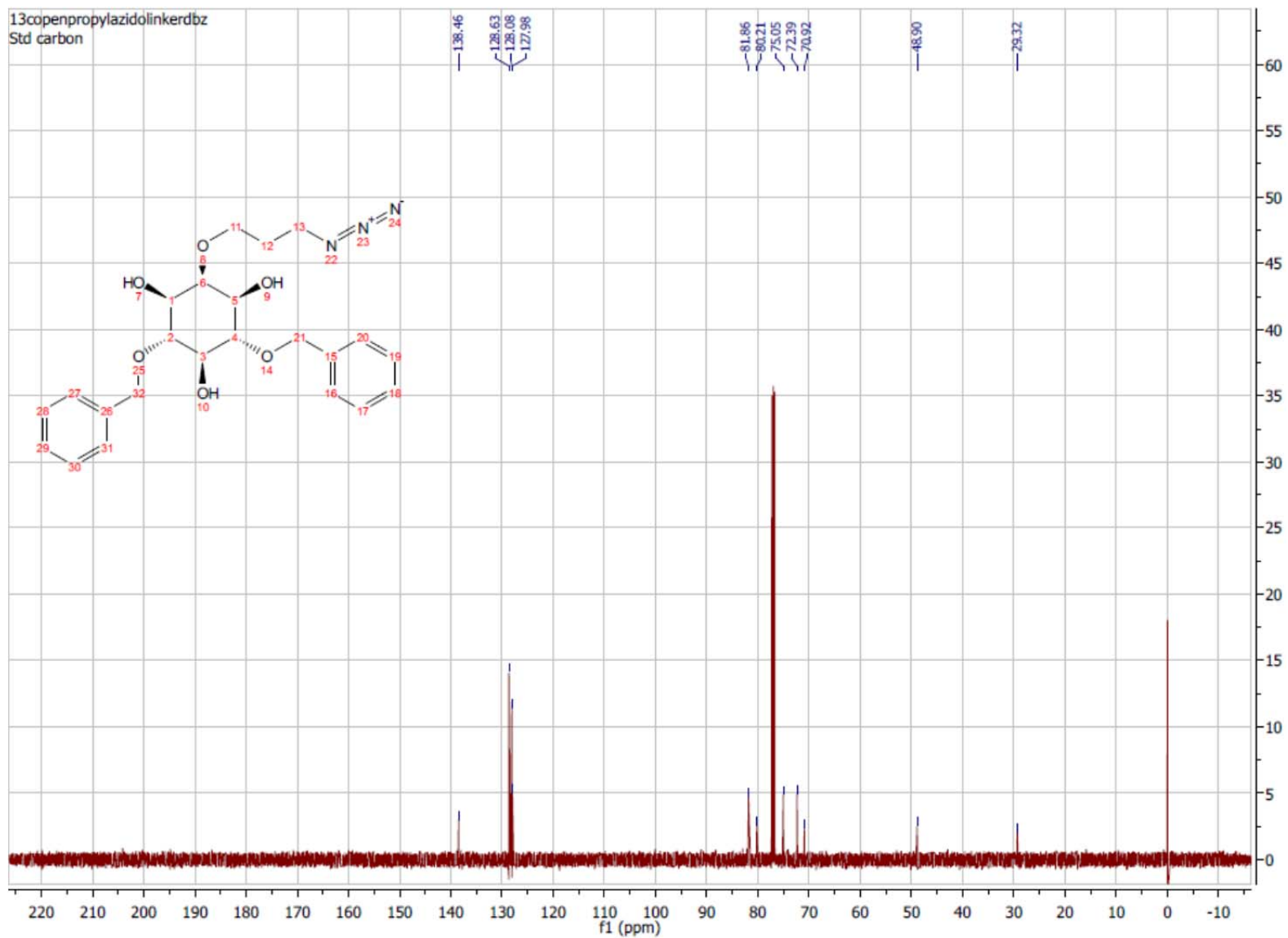
Operator Name: Tricks



¹H NMR of compound 5



¹³C NMR of compound 5

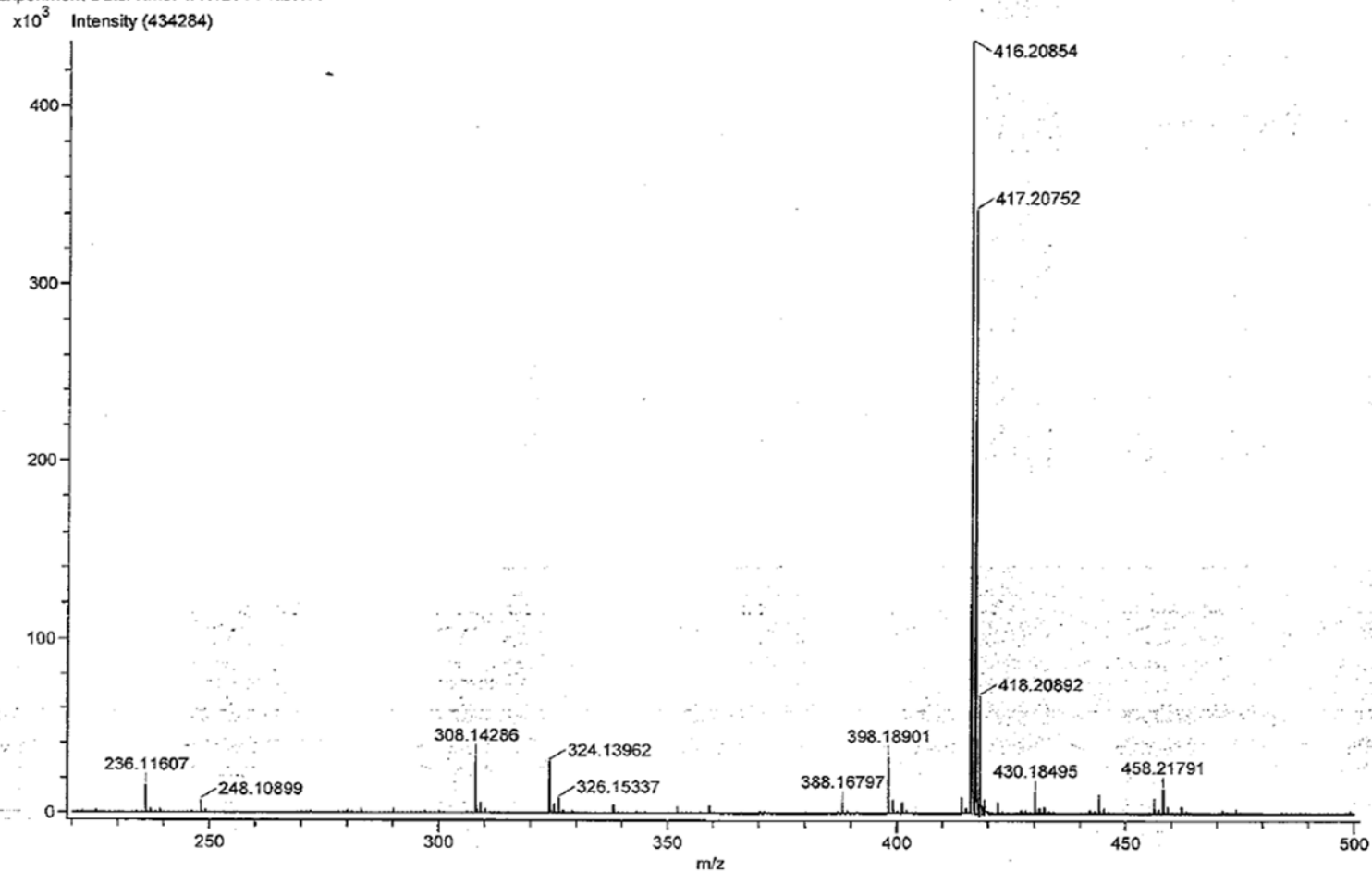


ESI-MS of compound 5

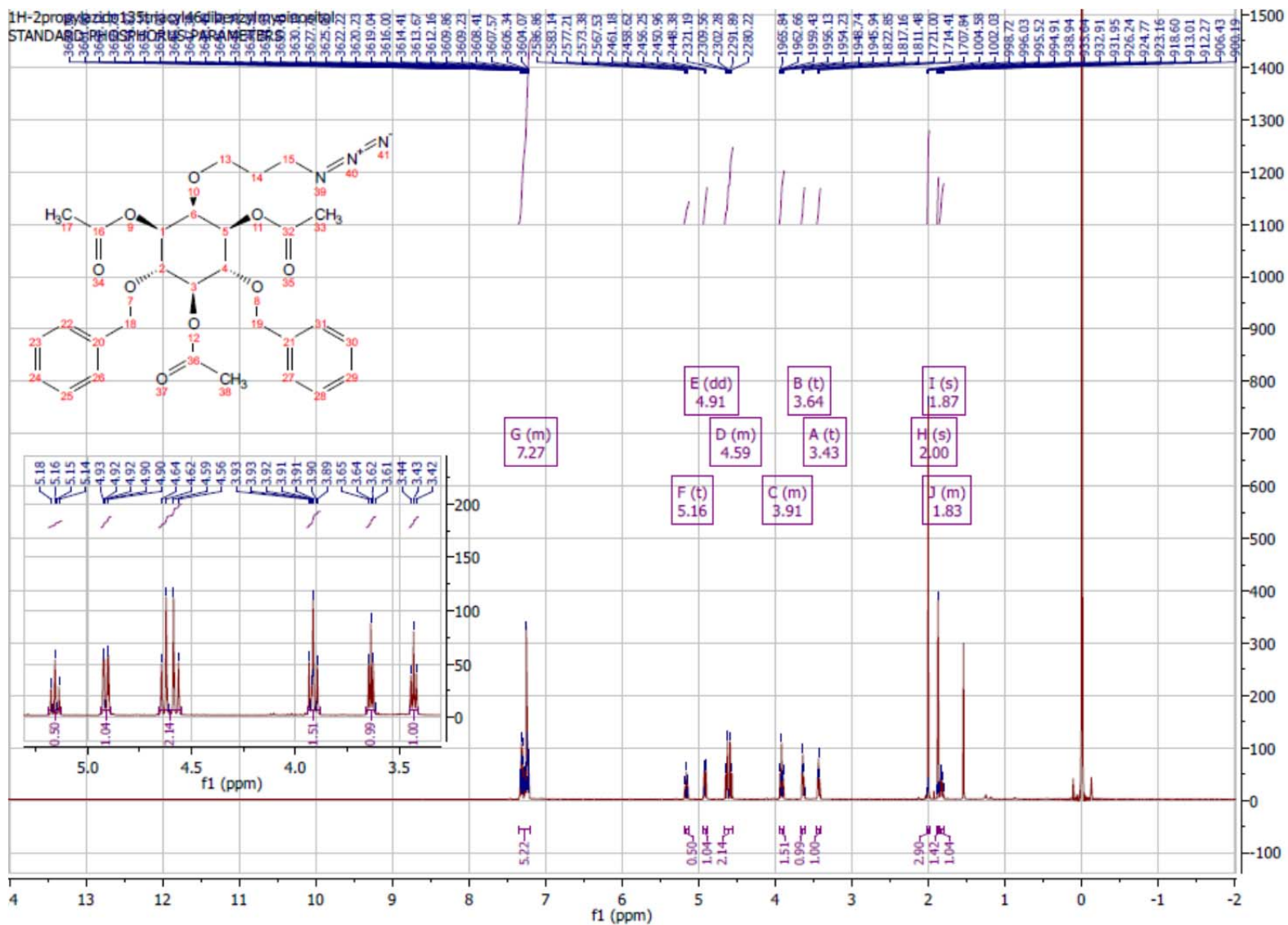
Acq. Data Name: 140117_Best_tricks_propylinkerdbz
Internal Sample Id:
Ionization Mode: ESI+ Orifice1 Volt Sweep: 30V
MS Calibration Name: PEG_DART_1000 Acquired m/z Range: 220.0..500.0
Reduction History: Correct Base[5.0%];Average(MS[1] 1.829..1.877)
Experiment Date/Time: 1/17/2014 1:20:20 PM

Spec. Record Interval: 1.0[s]
Ring Lens Volt: 10[V]
Time of Maximum: 1.859[min]

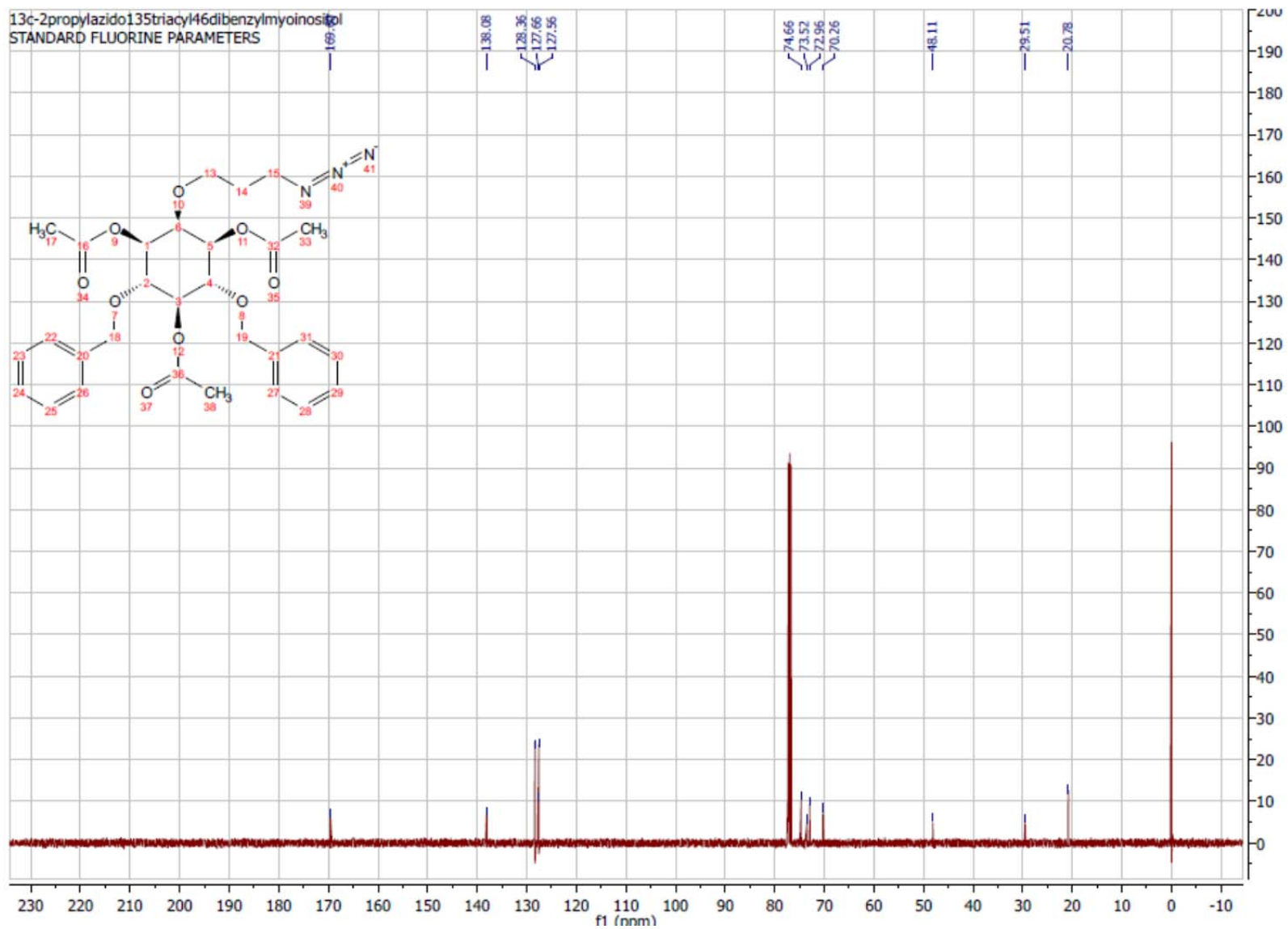
Operator Name: Tricks



¹H NMR of compound 6



¹³C NMR of compound 6



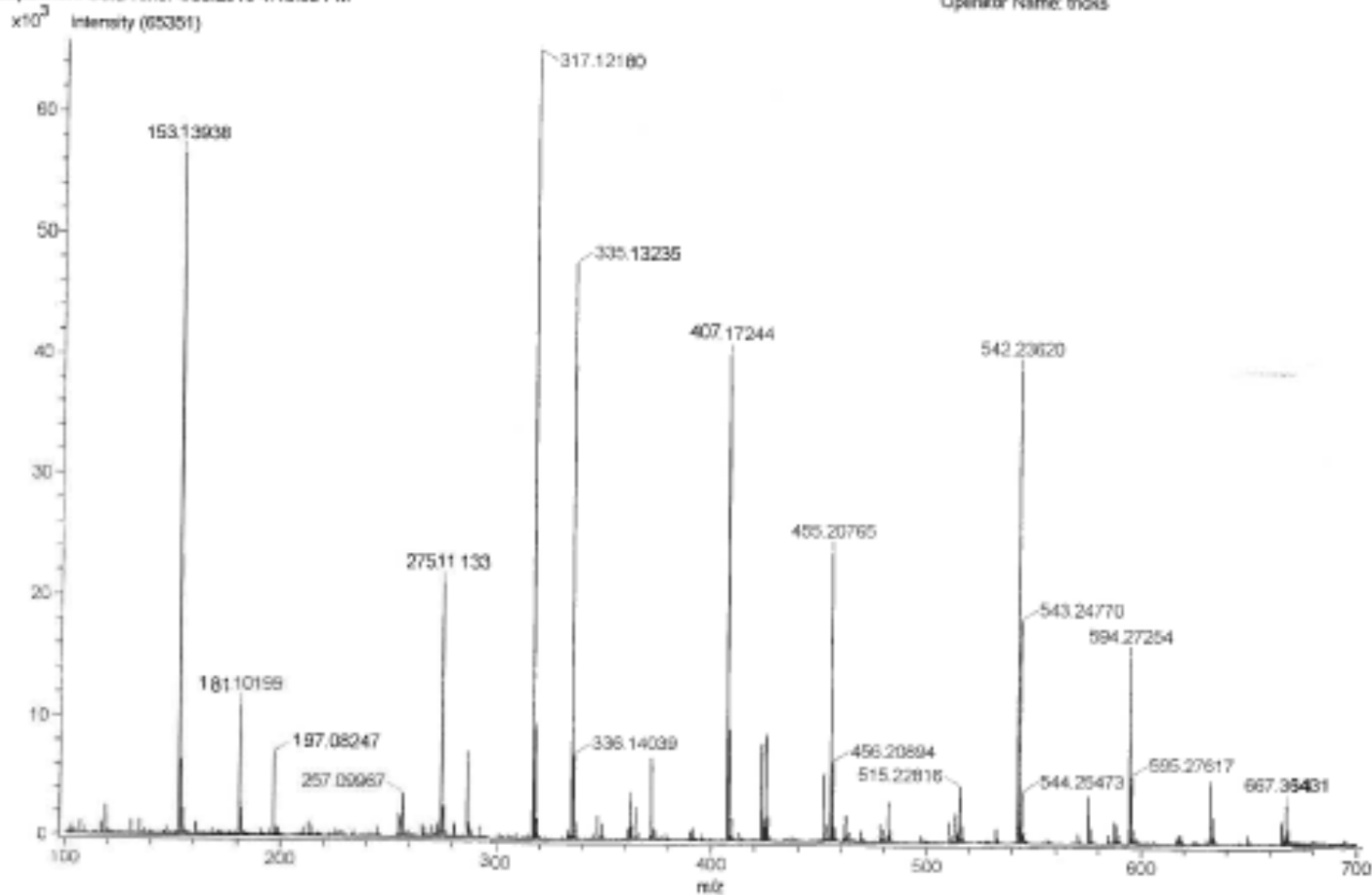
ESI-MS of compound 6

Acq. Data Name: 150430_Best_tricks_2propylazidod benzyltriacyltrycinoidol
Internal Sample Id:
Ionization Mode: ESI+
MS Calibration Name: DART(+)_1000
Reduction History: Correct Base[5.0%] Average[MS[1] 1.957_2.002]
Experiment Date/Time: 4/30/2015 4:43:00 PM

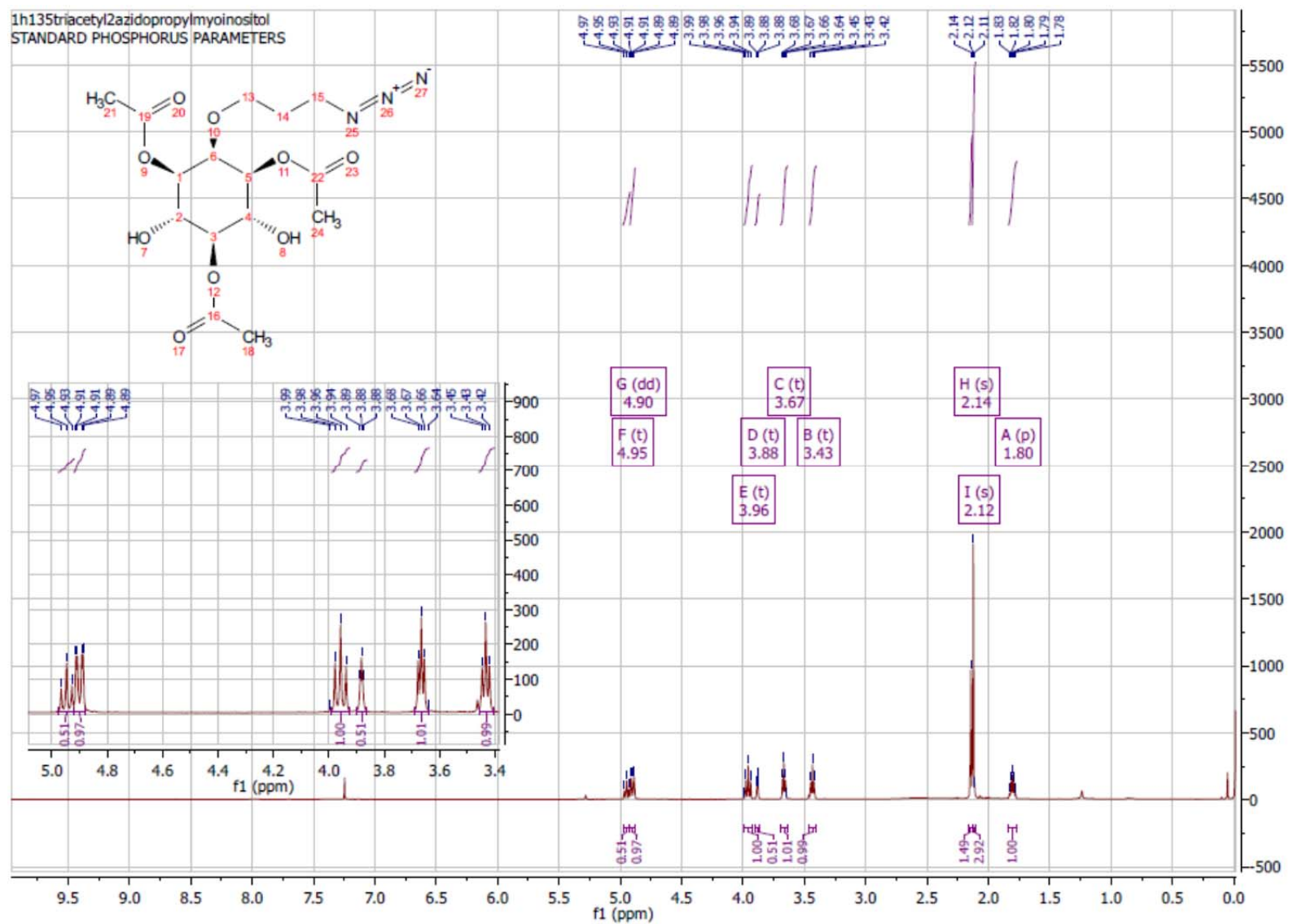
Orifice1 Volt Sweep: 15V
Acquired m/z Range: 100.0_700.0

Spec. Record Interval: 0.5(s)
Ring Lens Volt: 10(V)
Time of Maximum: 1.990(min)

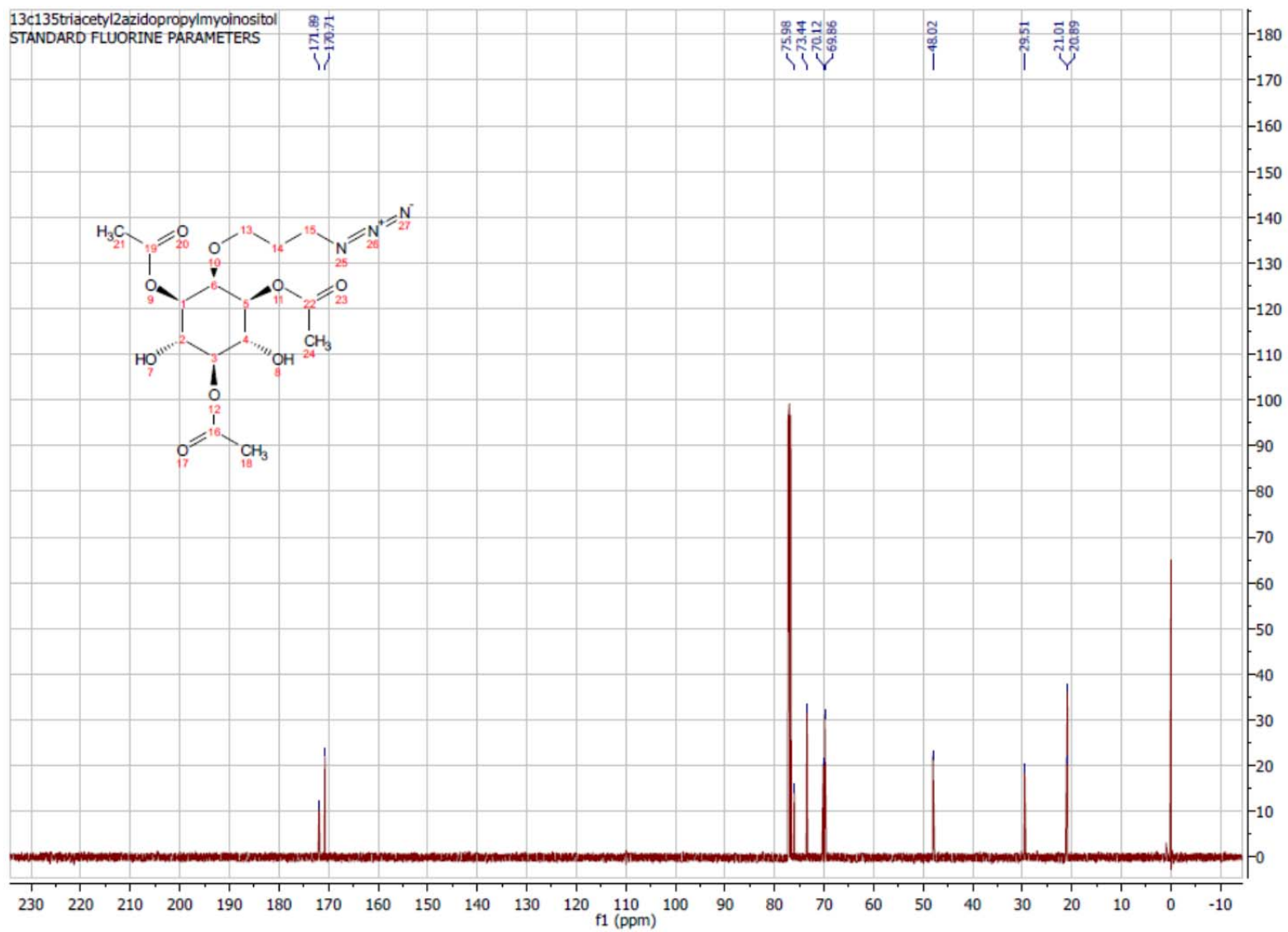
Operator Name: tricks



¹H NMR of compound 7



^{13}C NMR of compound 7



ESI-MS of compound 7

Acq. Date Name: 170816_best_tricks_13501acyl2propylazidomyo-inositol

Internal Sample Id:

Ionization Mode: ESI+

MS Calibration Name: DART(+)_1000

Reduction History: Correct Base(5.0%)/Average(MS(1) 0.576..0.638)

Experiment Date/Time: 8/16/2017 1:34:15 PM

Orifice1 Volt Sweep: 15V

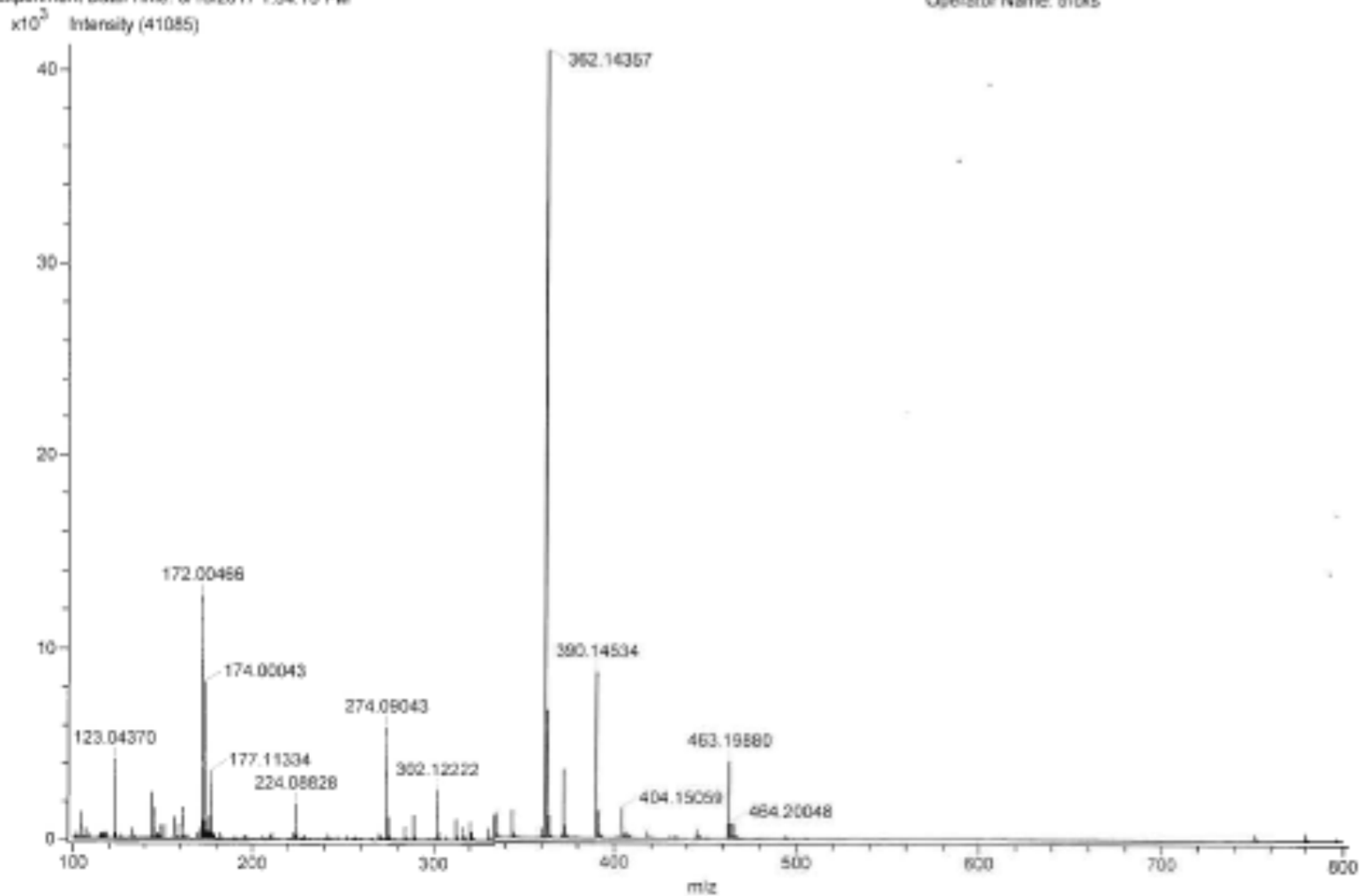
Acquired m/z Range: 100.0..800.0

Spec. Record Interval: 1.0(s)

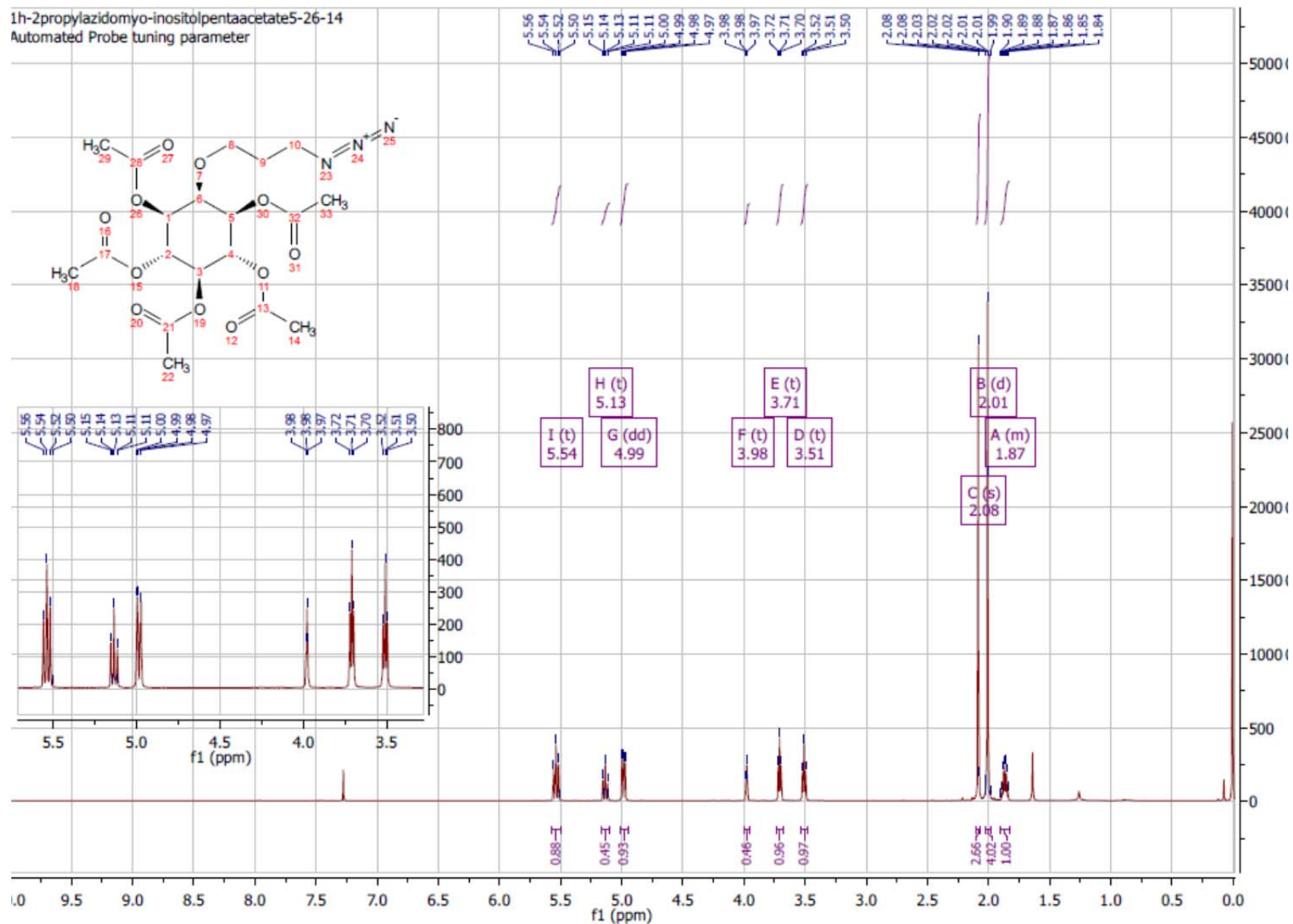
Ring Lens Volt: 10[V]

Time of Maximum: 0.610[min]

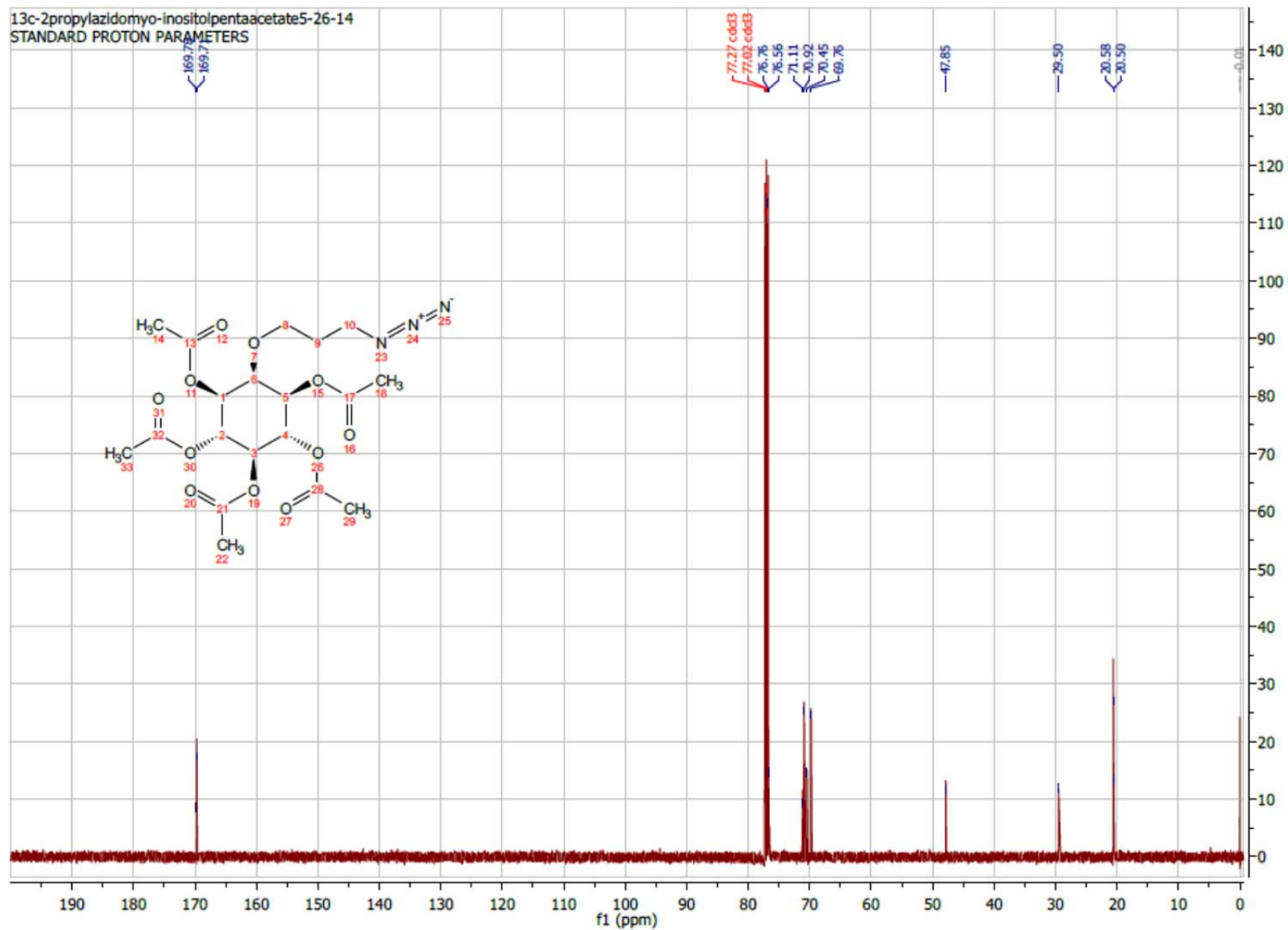
Operator Name: tricks



¹H NMR of compound 1b



¹³C NMR of compound 1b

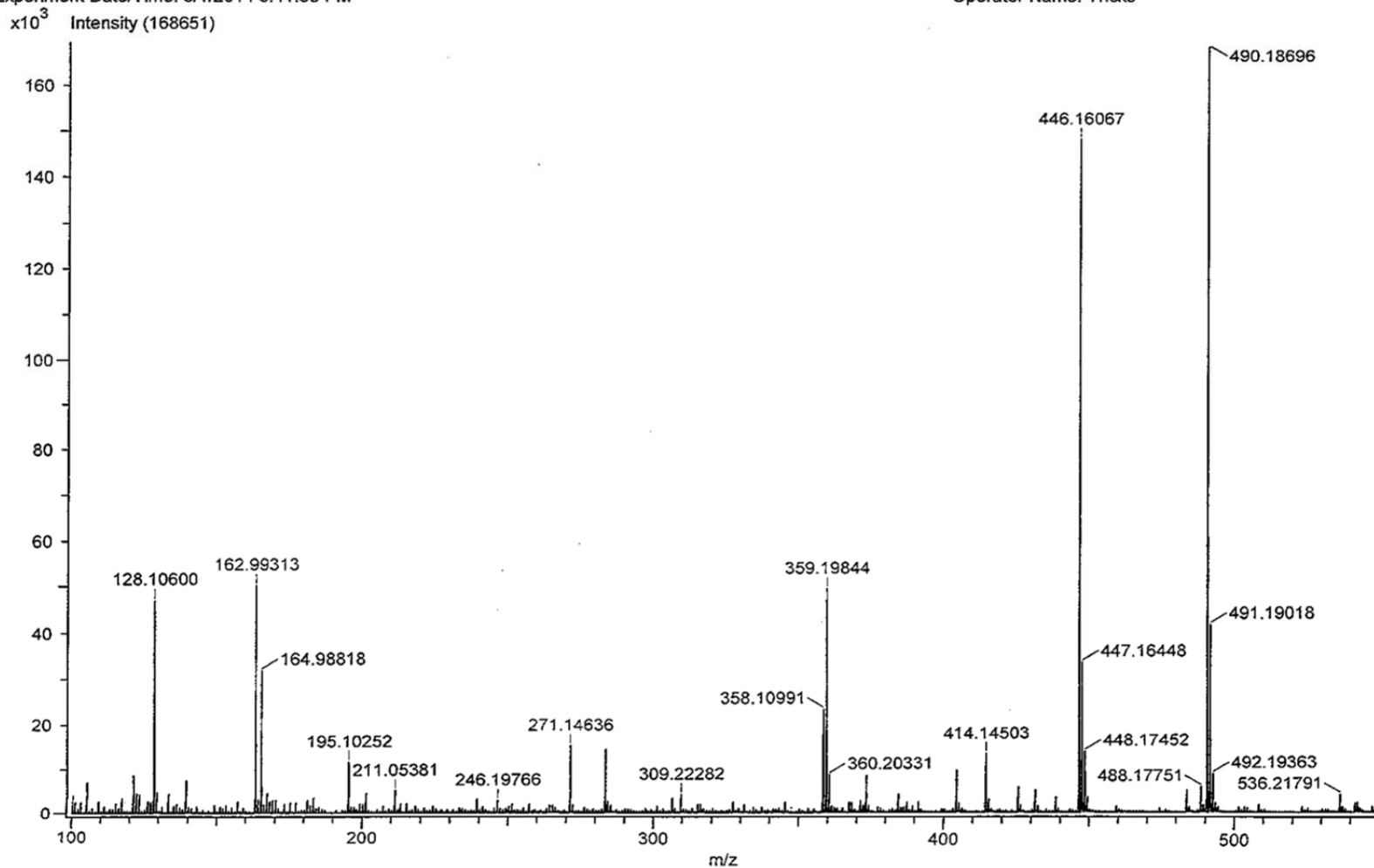


ESI-MS of compound 1b

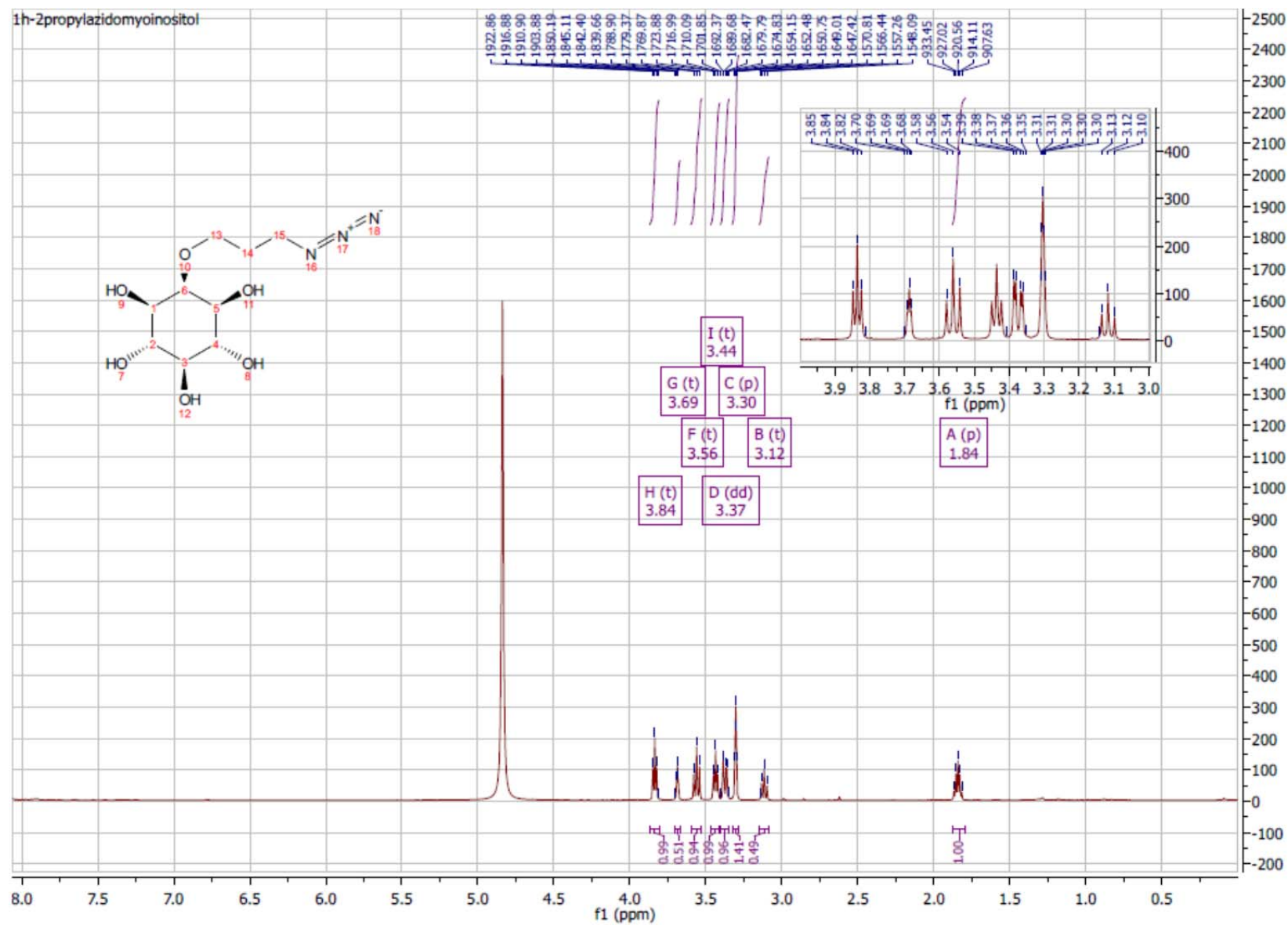
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Internal Sample Id:
Ionization Mode: ESI+ Orifice1 Volt Sweep: 30V
MS Calibration Name: PEG_DART_1000 Acquired m/z Range: 100.0..550.0
Reduction History: Correct Base[5.0%];Average(MS[1] 1.059..1.135)
Experiment Date/Time: 5/1/2014 3:41:58 PM

Spec. Record Interval: 1.0[s]
Ring Lens Volt: 10[V]
Time of Maximum: 1.098[min]

Operator Name: Tricks



¹H NMR of compound 1a



ESI-MS of compound 1a

Acq. Data Name: 160523_Best_tricks_propylazidomyoinositol
Internal Sample Id:
Ionization Mode: ESI+ Orifice1 Volt Sweep: 15V
MS Calibration Name: DART(+)_1000 Acquired m/z Range: 100.0..300.0
Reduction History: Correct Base[5.0%];Average(MS[1]) 1.083..1.132
Experiment Date/Time: 5/23/2016 3:39:47 PM

Spec. Record Interval: 1.0[s]
Ring Lens Volt: 10[V]
Time of Maximum: 1.115[min]

Operator Name: tricks

